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Professor Joshua Lederberg
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Dear Professor Lederberg:

I was quite delighted by your note and your interest in our work. Many thanks.

As to your questions:

1. Nitro compounds with the nitro group linked through nitrogen to carbon are usually reasonable shock stable (cf. TNT) and require, for example, the shock from detonation of a primary explosive (like lead azide) to set them off. It's when the nitro group is attached through a weak bond (e.g. O–N, as in nitroglycerine) that there's trouble. All the nitrocubanes we have prepared survive being hit with hammer! Nonetheless, we are always very cautious. (I am much embarrassed that I took off my safety glasses for the NY Times photo.) The Army has been able to purposefully detonate tetranitrocubane, apparently with spectacular results.

2. Hexanitrobenzene was first prepared quite a few years ago by the Russians. Their success was dismissed as cold war propaganda until they published the x-ray structure. After what I suppose what a lot of furious catch-up work, it turned out that HNB has no storage stability and hence was unsuitable for military use. There is apparently slow rearrangement to the nitrite ester of pentanitrophenol, which in turn is readily hydrolyzed by adventitious water to the phenol. (No doubt the Russians knew this before they published their synthesis.)

You might be interested to know that besides the expected shock insensitivity of octanitrocubane (ONC) there were numerous other reasons to predict that it would prove worth pursuing as a potential new explosive:

1. The heat of formation of cubane the hydrocarbon is *plus*144 kcal/mole. There is about 150 kcal/mole strain energy in the cage and this would contribute substantially (~15%) to the energy release on detonation. Interestingly, there are no "allowed"paths for cubane cleavage, so although the cage skeleton is thermodynamically a powerhouse, it is kinetically "a rock."

2. The oxygen balance in ONC is "perfect" ----> $8CO_2$ and $4N_2$

3. Cubane is one of the most dense hydrocarbons known (1.29 g/cc) and hence octanitrocubane can be predicted to be a very dense nitrocarbon. Density is supposedly crucial to performance: obviously, the more moles per limited shell volume the better; but more important the detonation pressure is taken (empirically) to go up with density squared.

The density of octanitrocubane is 1.979 g/cc. Interesting, heptanitrocubane has a higher density, 2.028, exceeded amongst C,H,N,O compounds only by one particular polymorph of CL-20. (Most nitro compounds are polymorphous.) In the crystal packing of heptanitrocubane an electron-rich oxygen of a nitro group of a neighbor molecule close-approaches (below van der Waal's distance) the electron deficient carbons of a fully-nitrated cubane face. Using crystallization under high pressure we think we can coax ONC into similar packing (calcd. density: 2.1 - 2.2 g/cc, by far the most dense C, N, O compound ever!). Unfortunately, we may never have the chance. After 20 years of supporting the project, the Army is disappointed that the present ONC density is slightly less than their much-hyped prediction. They are also worried about cost. Silly, as it's a matter that has never been addressed. Now that we know that ONC actually exists (once the crucial question) and that it is stable, we can logically go on to find methods to make it cheaply. Indeed, derived from the ONC synthesis, we now have most probably the methodology for the first synthesis of dinitroacetylene (a fascinating compound in its own right, but still unknown) and maybe we can bring about its direct tetramerization to ONC (calculated to be downhill by ~ 100 kcal/mole).

Anyhow, we have had lots of fun with the cubane system. I've taken the liberty of sending herewith a reprint of a review of its fundamental chemistry, much of which was discovered during the quest for ONC. I've also included a copy of the reprint you requested.

Thanks again for your interest. Maybe you can drum up some interest at DARPA. We'd love to continue our work, but the funding situation looks dismal.

With regards,

Phil Eaton